

3E-hexenol-d2

Inchi:	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h3-4,7H,2,5-6H2,1H3/b4-3+/i1D2
InchiKey:	UFLHIIWVXFIJGU-UVWCYZJASA-N
Formula:	C6H10D2O
SMILES:	CCC=CCCO
Mol. weight [g/mol]:	102.17

Physical Properties

Property code	Value	Unit	Source
gf	-56.96	kJ/mol	Joback Method
hf	-202.18	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.335		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
ripol	1367.00		NIST Webbook
tb	433.02	K	Joback Method
tc	601.76	K	Joback Method
tf	213.12	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.78	J/molxK	433.02	Joback Method
cpg	200.94	J/molxK	461.14	Joback Method
cpg	209.69	J/molxK	489.27	Joback Method
cpg	218.06	J/molxK	517.39	Joback Method
cpg	226.05	J/molxK	545.51	Joback Method
cpg	233.69	J/molxK	573.64	Joback Method
cpg	240.99	J/molxK	601.76	Joback Method
dvisc	0.0918576	Paxs	213.12	Joback Method
dvisc	0.0156415	Paxs	249.77	Joback Method

dvisc	0.0041899	Paxs	286.42	Joback Method
dvisc	0.0015133	Paxs	323.07	Joback Method
dvisc	0.0006726	Paxs	359.72	Joback Method
dvisc	0.0003473	Paxs	396.37	Joback Method
dvisc	0.0002006	Paxs	433.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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